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The College of William and Mary

Williamsburg, Virginia 23185

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ATMOS Spacelab I Science Investigation

Mary Ann H. Smith
Research Associate

Jae H. Park
Research Assistant Professor

Research Summary

Research Title: ATMOS SPACELAB I SCIENCE INVESTIGATION

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Investigators: PI: Dr. Jae H. Park, College of William and Mary, Williamsburg, Virginia 23185 (804)827-2576

CO-I: Dr. Mary Ann H. Smith, College of William and Mary, Williamsburg, Virginia 23185 (804)827-2576

CO-I: Dr. Jerold T. Twitty, Systems and Applied Services Corporation, Riverdale, Maryland 20840 (804)827-2576

CO-I: Dr. James M. Russell III, NASA Langley Research Center, Hampton, Virginia 23665 (804)827-2576

Description of Research and Results:

Analysis of existing infrared spectra from JPL's Mark I High Speed Interferometer (HSI) balloon flights (1976, 1977) and development of analysis techniques applicable to similar data from HSI Mark II balloon flights (1979) and from the ATMOS experiment (Spacelab III). Specific techniques under development include line-by-line simulation of the spectra to aid in the identification of absorbing gases, simultaneous retrieval of pressure and temperature profiles using carefully chosen pairs of CO_2 absorption lines, and the use of these pressures and temperatures in the retrieval of gas concentration profiles for many absorbing species. A search for new absorption features was also carried out, and special attention was given to identification of absorbing gases in spectral bandpass regions to be measured by the Halogen Occultation Experiment (HALOE).

Future Plans:

The temperature and pressure inversion and gas concentration inversion algorithms will be further developed and refined, and will be used to retrieve profiles from the Mark I data and from the Mark II data to become available in late 1979. The search for new absorption signatures in the Mark I and Mark II spectra will continue, leading to the determination of actual amounts or upper limits for the stratospheric concentrations of $CH_3C\ell$, $CH_3CC\ell_3$, H_2CO and OCS. More efficient techniques for line-by-line simulation of the spectra will also be explored.

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I. INTRODUCTION

The primary purpose of the proposed research has been to analyze existing high-resolution infrared spectra measured by JPL's Mark I High Speed Interferometer (HSI) in balloon-borne solar occultation experiments (1976 and 1977), and to develop analysis techniques applicable to similar data from the Mark II instrument to be flown on a balloon in mid-1979 and data from ATMOS, which is now scheduled to fly on Spacelab III (1982). The specific objectives of the current study include identification of major absorbers in the Mark I spectra, simulation of the absorption spectra using a line-by-line method for comparison to the measured spectra, development of inversion techniques to obtain pressure and temperature profiles from CO_2 absorption lines, and the use of these pressures and temperatures in the simultaneous retrieval of various gas concentrations, focusing primarily on the gases and spectral regions important for HALOE (Halogen Occultation Experiment). Unknown features in the existing spectra were also to be identified and studied in more detail, with specific attention being given to the spectral region of the ν_4 band of $CH_3C\ell$. In the following pages of this report, the above-mentioned objectives will be discussed individually, describing both the current status of the research and the work planned for the future in each of these areas.

II. INVESTIGATIONS

1. Identification of Major Absorbers

Selected wavelength regions of HSI Mark I spectra from two different balloon flights (Texas, 1976 and Australia, 1977) are available in graphical form, and the complete spectra are stored in digital form on magnetic tape. With the help of the Atlas of Infrared Absorption Lines (NASA CR-2925) published at NASA Langley Research Center, as well as additional data on methane (CH_4) provided by Dr. Toth at JPL, features belonging to the major absorbing gases (H_2O, CO_2, O_3, CH_4, N_2O) are readily identified in the graphical spectra. A spectral plotting program, derived from one developed by R. Norton and B. Stedry at JPL, allows the display of spectral data with a scale and resolution chosen by the user (Fig. 1). Coupled with the line-parameter plotting program used to generate the Atlas (Fig. 2), the spectral plotting program facilitates the identification of a large number of absorption features in the Mark I spectra.

2. Simulation of the Spectra

A multi-gas version of the line-by-line model developed by Drayson (1966) has been used to simulate several regions of the HSI Mark I spectra (Fig. 3). The model has been modified to include the effects of the real instrumental line shape for the interferometer, and a faster routine to calculate the Voigt line shape (Drayson, 1976) has been included. Parameters in the model can be easily changed in order to simulate the high-resolution Mark II spectra when they become available. The agreement between the simulated spectra and the measured spectra is quite good. The remaining discrepancies are almost entirely due to the amounts of gases assumed in the model,

filter effects present in the measured spectra, and, in some spectral regions, missing or uncertain line parameters input into the model. The computational efficiency and speed of the model, running on the CDC 6600 computer, have been improved, but the total cost of the simultations remains high. An alternative and more efficient simulation technique, based on the Fourier-Transform method of Dr. Mankin at NCAR, which runs on the STAR computer at LaRC, has been successfully used in LIMS data analysis at this center. This FFT model will be tested and evaluated for use in simulating HSI and ATMOS spectra.

3. Pressure and Temperature Sensing Using CO_2 Lines

In order to obtain gas concentration profiles in a limb-viewing experiment, it is desirable to get temperature and pressure profiles directly from spectral data rather than relying on climatological data and tangent heights calculated from instrument pointing information. We have begun developing an iterative technique for simultaneous retrieval of pressure and temperature profiles using a pair of CO_2 absorption lines having different lower-state energies, but appearing in the same spectrum. Investigation of the temperature and pressure dependence of CO_2 line strengths has indicated that lines having lower-state energies on the order of 0 -800 cm^{-1} are best suited for pressure-sensing, while those with lower-state energies greater than 1000 cm^{-1} are most strongly temperature-dependent. A technique for temperature sensing using isolated CO_2 lines in the HSI spectra has already been developed by Toth (1977), and pressures may be retrieved using a curve-of-growth method (Park et al 1979), provided that equivalent widths of the individual CO_2 lines or a group of lines can be determined with sufficient accuracy. A numerical algorithm where the retrieved temperature and pressure profiles are used to correct each other in successive iterations has recently been written and has been tested using simulated equivalent width values.

Figures 4 and 5 show the expected error in temperature and pressure for a single atmospheric layer, retrieved using the above-mentioned algorithm. As predicted from analysis of line-strength temperature and pressure dependence, the highest accuracies in retrieved temperatures are achieved for CO_2 lines having lower-state energies greater than 1000 cm^{-1}. For the case shown in Fig. 5 where we assume that the temperature profile is known perfectly ($\Delta T = 0$), the error in retrieved pressure does not appear to vary with the lower-state energy of the CO_2 line chosen for pressure sensing. When uncertainty ΔT is included in the temperature profile, the pressure uncertainty Δp remains small for CO_2 lines having lower-state energies less than 600 cm^{-1}. Accuracies for both pressure and temperature retrievals deteriorate when the absorption line is very weak (absorption less than 10%) or nearly saturated (absorption greater than 95%). The error analyses in Figs. 4 and 5 were carried out for a rather low atmospheric pressure, 0.7 mb, which corresponds to an altitude of 50 km. We have found that the accuracy of both the pressure and temperature retrievals for higher atmospheric pressures is considerably better than the results shown in the figures.

Testing and further development of the pressure and temperature retrieval algorithm will continue, making use of equivalent widths of CO_2 lines measured in the HSI Mark I spectra. There is also under development a program which will automatically scan the HSI spectra stored on magnetic tape, find the centers of spectral lines and calculate their equivalent widths. The line-finding and equivalent width routines are based on the DERPTH program written by H. Delouis at the Centre National de la Recherche Scientifique, Orsay. Eventually these routines will be incorporated, along with the atlas and spectral ratio and plotting programs, into a software library for analysis of HSI and ATMOS data at LaRC.

4. Simultaneous Retrieval of Gas Concentrations

Several methods for retrieval of gas concentrations hav been studied, among them the direct curve-of-growth method, which requires accurate determination of equivalent widths, iterative simulation and fitting of line profiles,

and the equivalent-width-ratio method used by Farmer and Raper (1977). An algorithm for inversion of a gas concentration profile using the single-line curve of growth method combined with Drayson's "onion peeling" technique has been written and is currently being tested. Further development and testing of gas-concentration retrieval methods will proceed in parallel with the work on the temperature and pressure retrievals and automatic calculation of equivalent widths. In addition, selection of absorption lines that can be used for most accurate retrieval of concentrations of stratospheric minor gases will be carried out.

5. Support for HALOE

Work done as part of the current investigation has contributed to the support of HALOE, aiding in identification of the best spectral regions in which to detect each of the gases of interest ($HC\ell$, HF, CH_4, NO, H_2O, and CO_2). Detailed analysis and line identification in each of the chosen spectral regions remains to be done, particularly in regard to the identification of solar lines. Line-by-line simulations have already been carried out for each of these regions, and the pressure, temperature and gas concentration retrieval algorithms under development in this investigation will be applied first to the HALOE spectral regions. The gas concentration profiles determined from the HSI spectra will be used to refine previous sensitivity analyses for HALOE. Retrieval of $HC\ell$ mixing-ratio profiles will receive high priority because the HALOE brassboard instrument for the $HC\ell$ channel will be test-flown on the CV990 in the summer of 1979. Since both the ATMOS and HALOE instruments are now scheduled to fly on Spacelab III, there will be a unique opportunity for comparison of gas concentration profiles determined from the two experiments.

6. Line Identification and Search for New Signatures

An extensive analysis and search for new signatures has been carried out for the spectral region between 3055 and 3075 cm^{-1}. Attention was focused on this region to determine if absorption features belonging to the ν_4 fundamental of methyl chloride ($CH_3C\ell$) were detectable in the HSI Mark I spectra. By comparison of the real spectra with Atlas line data and simulated spectra, there was found a broad, weak absorption feature extending between 3062 and 3072 cm^{-1}, which appears in the Texas spectra but not in the Australian data. Several species including H_2O, CO_2, O_3 and CH_4 have been ruled out as the cause of this feature. Simulations of $CH_3C\ell$ absorption in this region, assuming its stratospheric mixing ratios to be one to ten times the values calculated by Crutzen et al (1978), seem to indicate that methyl chloride alone could not account for the broad envelope found in the Texas spectra. The 3μm absorption spectra of other halogenated hydrocarbons, including methyl chloroform ($CH_3CC\ell_3$), are now being studied and compared to the Mark I data in an effort to make a definite identification of the broad feature. Upper limits on the stratospheric concentrations of $CH_3C\ell$, $CH_3CC\ell_3$ and other halogenated hydrocarbons will be calculated after the identification of the broad feature is made.

Preliminary surveys of the Mark I spectra to search for the signatures of Freon-14 (CF_4), formaldehyde (H_2CO) and carbonyl sulfide (OCS) have also been carried out. Since the strong ν_3 and ν_4 absorption bands of CF_4 lie outside the bandpass of the filters used in the Mark I balloon flights, we cannot determine anything about CF_4 concentrations from this data. Formaldehyde and carbonyl sulfide have strong absorption bands at 3.5μm and 5μm (see Fig. 1),

respectively, which have not been detected in the Mark I spectra through visual inspection. However, careful analysis of the spectra in these regions and simulations of the spectra based on accurate laboratory data may reveal weak absorption by OCS or H_2CO in these two regions and allow the determination of gas concentrations or upper limits for these stratospheric trace species.

III. SUMMARY

Considerable progress has been made this year in a number of the research areas specified in the objectives of this study. Identification of absorption features belonging to major infrared-active atmospheric constituents in any region of the Mark I spectra is accomplished readily by the use of both the Atlas and spectral plotting programs. The line-by-line simulation model operating on the CDC 6600 computer has been made as efficient as possible, and the less costly FFT model running on the STAR computer may be used for simulation of HSI data in the near future. Algorithms for the combined retrieval of pressure and temperature profiles using CO_2 lines and for the retrieval of gas concentrations have been outlined, and early versions of numerical routines for these retrievals have been tested. A new absorption feature in the 3.3μm region has been found in the Texas data, but is not yet identified. Preliminary surveys of the spectra have also been carried out in preparation for the determination of upper limits on the stratospheric concentrations of $CH_3C\ell$, $CH_3CC\ell_3$, H_2CO and OCS. The work on pressure, temperature and gas concentration retrievals will be emphasized in the coming year, in support of HALOE flight experiments.

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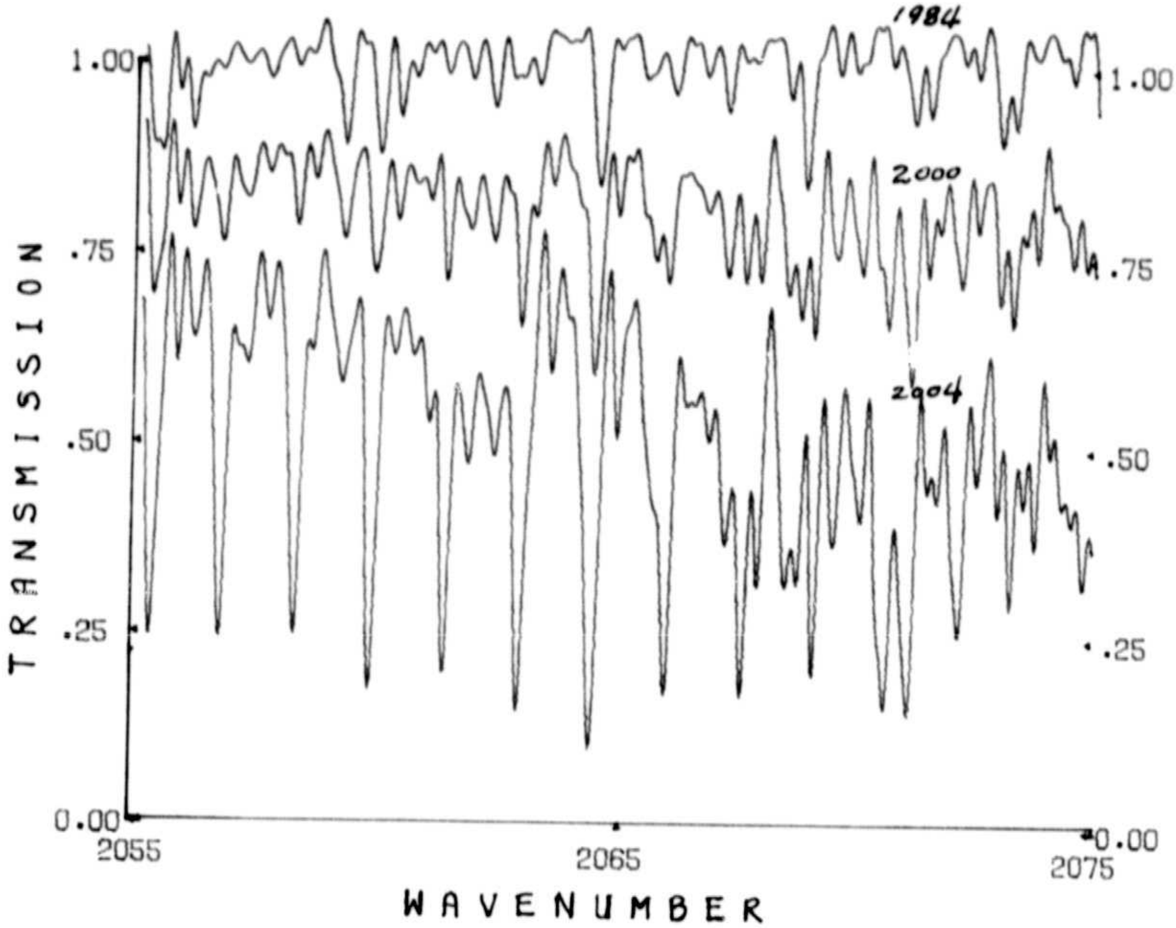
LIST OF FIGURES



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2004
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.50
.25
0.00
TRANSMISSION
2055
2065
2075
WAVENUMBER

Fig. 1

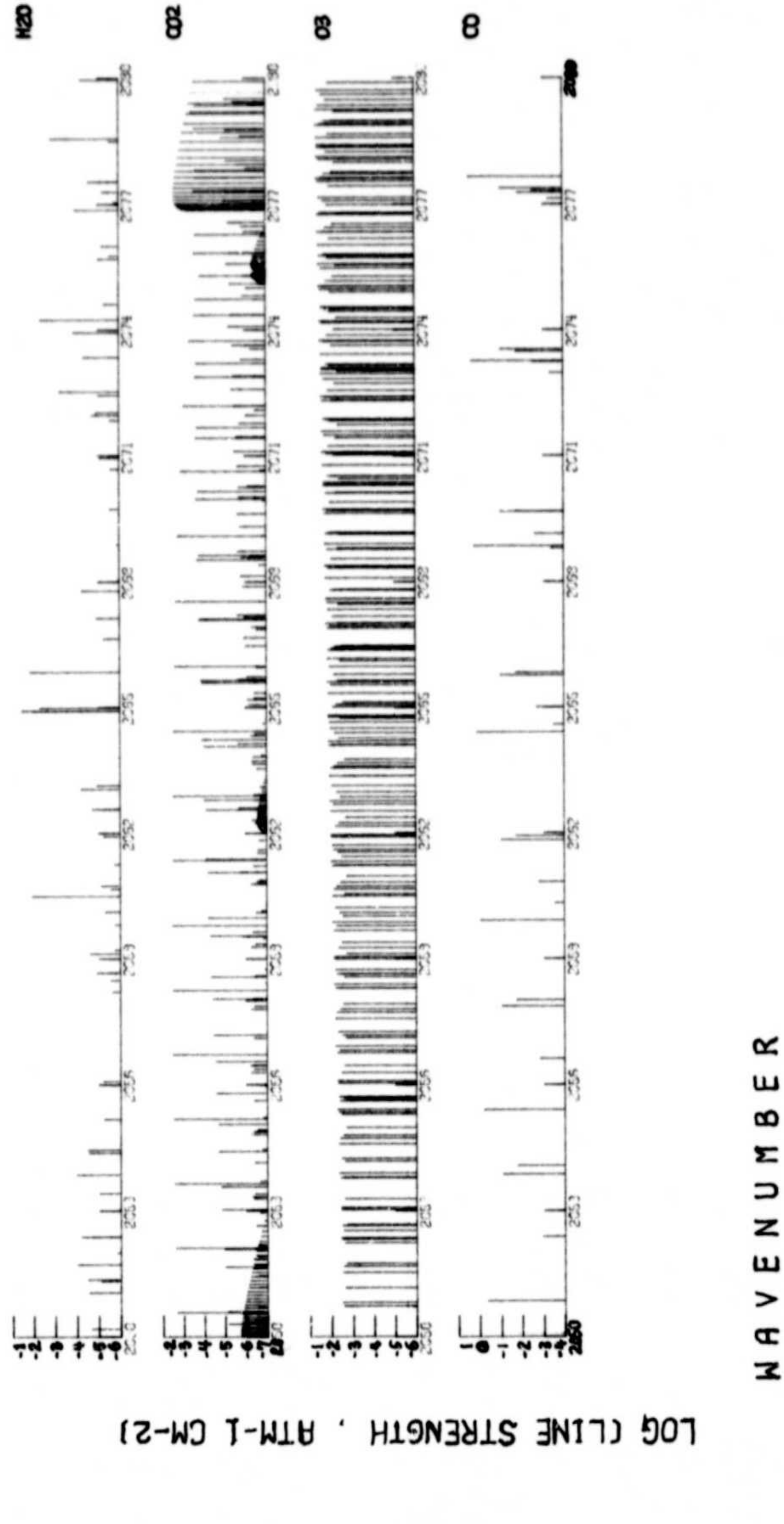
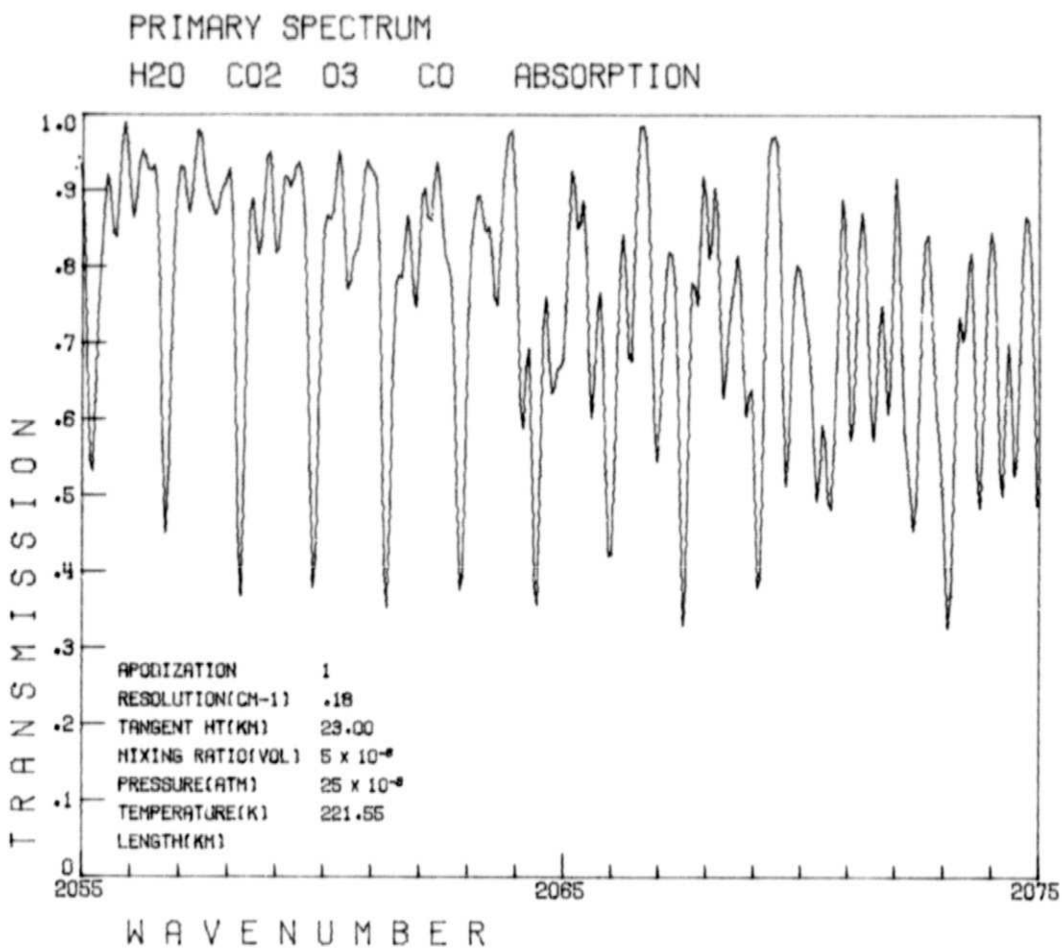


Fig. 2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.7
.6
.5
.4
.3
.2
.1
0
TRANSMISSION
APODIZATION 1
RESOLUTION(CM-1) .18
TANGENT HT(KM) 23.00
MIXING RATIO(VOL) 5 x 10
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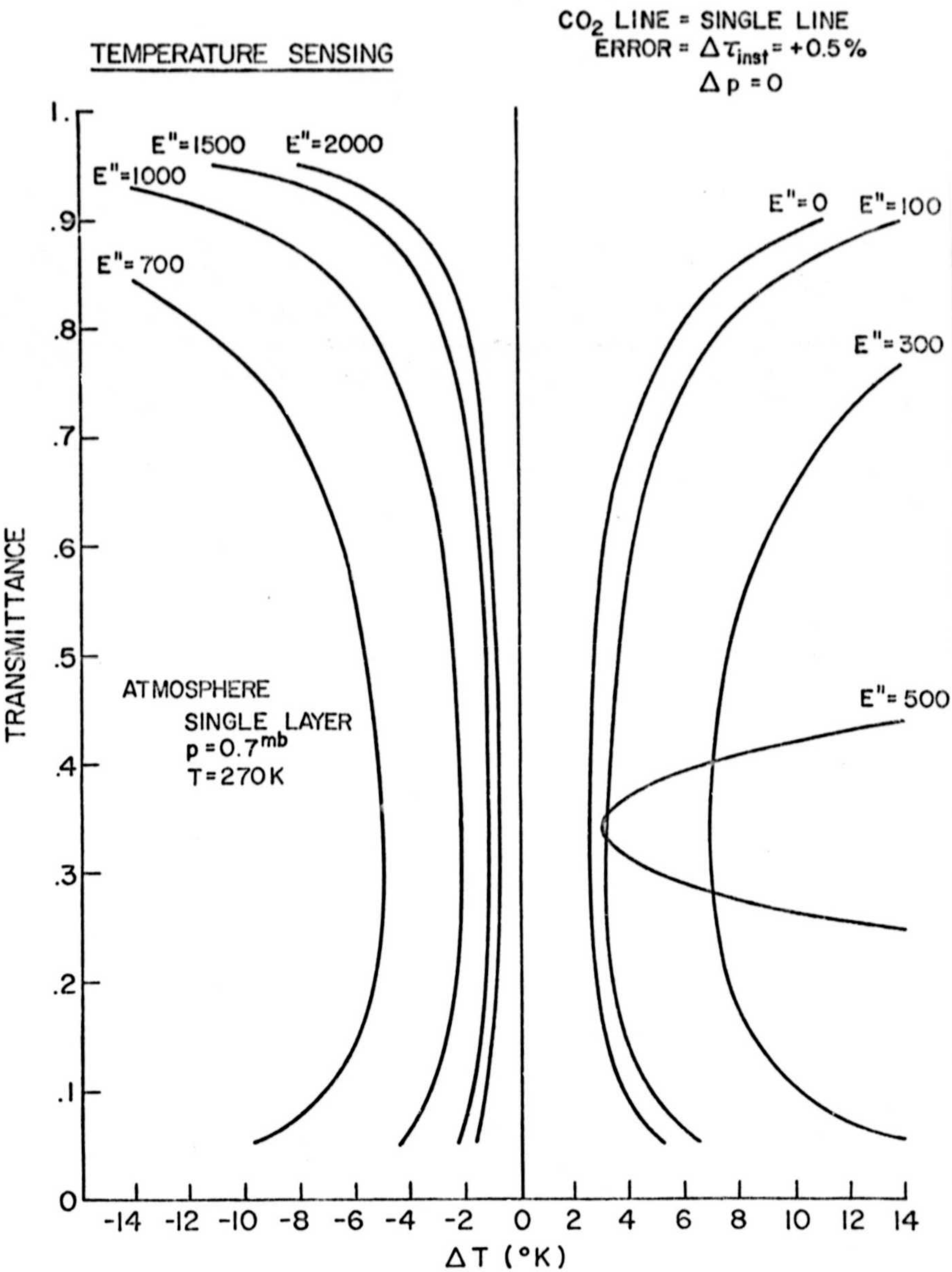
LENGTH(KM)
2055
2065
2075
WAVENUMBER

Fig. 3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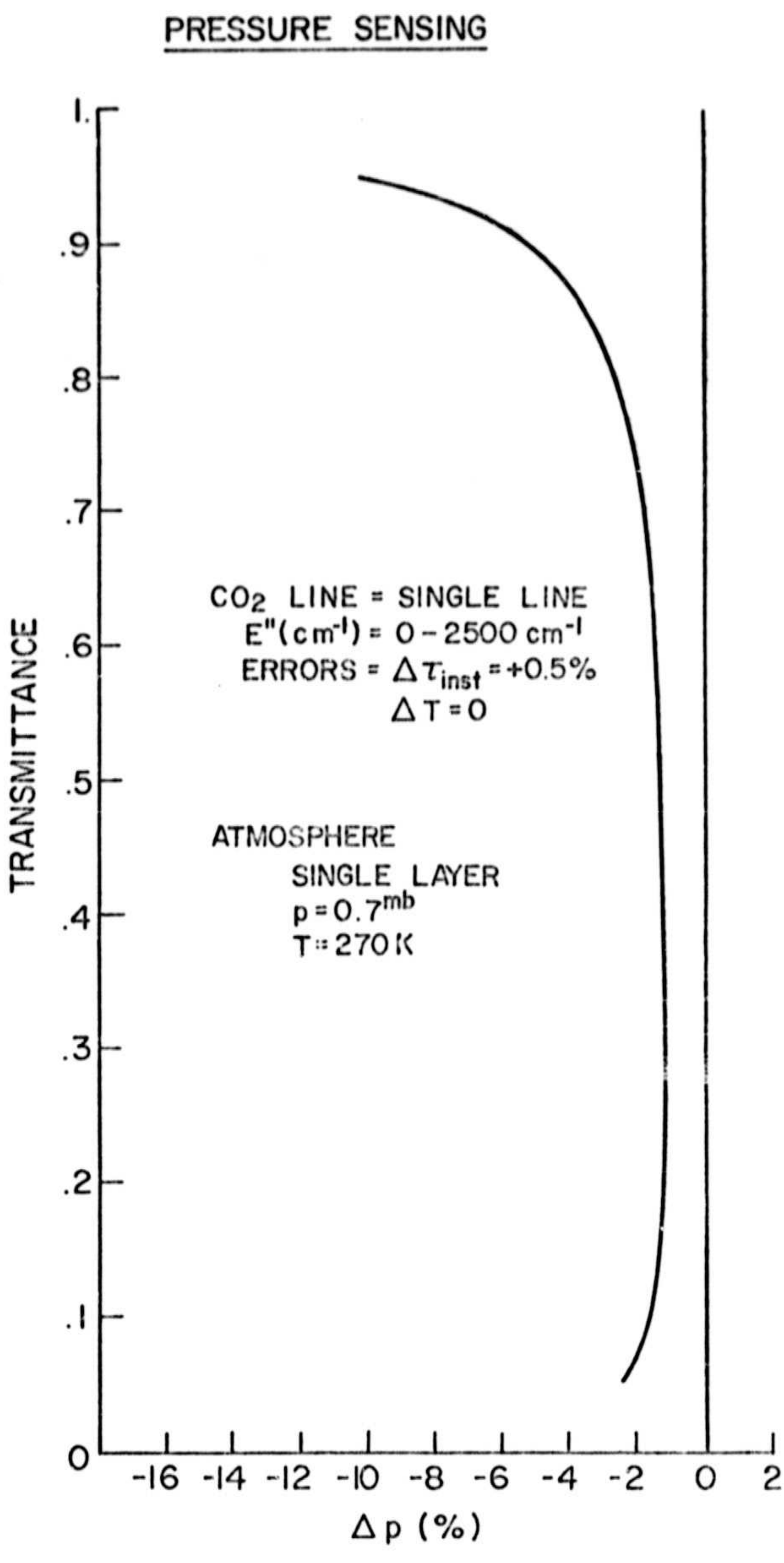
Δp = 0
E"=1500
E"=2000
E"=1000
E"=700
E"=0
E"=100
E"=300
E"=500
ATMOSPHERE
SINGLE LAYER
p = 0.7 mb
T = 270 K
TRANSMITTANCE
ΔT (°K)

Fig. 4



PRESSURE SENSING
TRANSMITTANCE
1.
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.7
.6
.5
.4
.3
.2
.1
0
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Δ p (%)
CO_2 LINE = SINGLE LINE
E"(cm^{-1}) = 0 - 2500 cm^{-1}
ERRORS = $\Delta\tau_{inst}$ = +0.5%
$\Delta T = 0$
ATMOSPHERE
SINGLE LAYER
p = 0.7^{mb}
T = 270 K

Fig. 5